3D Simulation of Material Deposition

presentation to

SRC/Material and Process Sciences/Back End Process TAB
Rensselaer Polytechnic Institute

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Los Alamos National Laboratory

28 October 1999

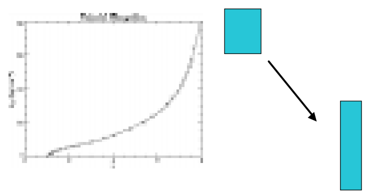
Outline of Talk

- Introduction / Motivation
- Atomistic Simulations
  - Copper on Copper
  - Argon on Copper
- TopoSim-3D
  - capabilities
  - examples

From the Molecular to the Macro Scale

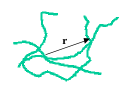
Stress/Strain

Uniaxial Elongation



Molecular theory

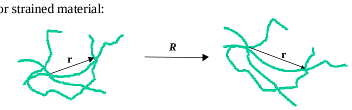
- Ingredients:
  - Assume a network model.



  - Distribution of chain lengths:
    - f_N: probability of finding a chain with N monomers between two adjacent nodes in the network,
    - $\rho^{(N)} = \rho_c\, f_N$: distribution of chains of length N.
  - Distribution of polymer chain orientations in the unstrained material:
    - $P_{eq}^{(N)}(\mathbf{r})$.

Molecular theory

- For strained material:



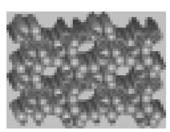
  - Distribution of polymer chain orientations in strained material:
    - $P^{(N)}(\mathbf{r}, R)$.
- Use equilibrium statistical mechanics.

Catalysis

Modeling of acidity in zeolites

A. Redondo and P.J. Hay, *J. Phys. Chem.* 97, 11754 (1993)

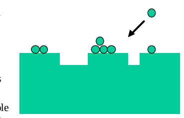
- Zeolite ZSM-5 (MFI)
  - Aluminum atoms substitute a small number of silicons
  - 12 different tetrahedral sites for aluminum
- Electronic structure calculations using clusters
- "Cut" a cluster from the crystal and saturate dangling bonds with OH groups
  - A different cluster for each tetrahedral site
- Include second nearest neighbors in the cluster
  - 96 to 125 atoms



Film Growth

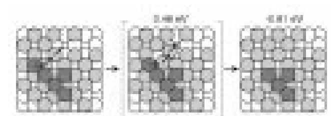
Motivation

- Many materials problems are amenable to atomistic simulation but are not viable with current hardware and software when there is a coupling between different temporal scales.
- Example: film or crystal growth
  - Deposition impact events are very quick (~1 ps)
    - Can use molecular dynamics
  - Time between deposition events is much longer (~1 ms)
    - Molecular dynamics unfeasible (limited to times of order 100 ns)
  - Diffusion and reorganization events control the morphology of the epitaxial growth layers
    - Need some other method for diffusion processes



3-atom concerted event during surface smoothing Ag/Ag(100)

- Hyperdynamics + parallel replica dynamics
- Three atoms move "simultaneously" in concerted mechanism
- Too complex for *a priori* inclusion in Kinetic Monte Carlo method



From the Molecular to the Macro Scale
Applications to Semiconductor Issues

- *As feature sizes decrease, it becomes increasingly necessary to understand how interactions at the atomic and molecular scale manifest themselves as bulk material properties*
- *The 1999 National Technology Roadmap for Semiconductors identifies several difficult challenges in modeling and simulation that face the industry in the near-to-long-term time frame.*

Difficult Challenges	Summary of Issues *(being addressed by National Labs)*
• Model thin film and etch variation across die/wafer	• Reaction paths, rates, plasma models, equipment/feature scale links
• Model new interconnect materials and interfaces	• Grain structure, diffusion barriers
• Atomistic process modeling	• Accurate models for process integration

TopoSim-3D

A Three-Dimensional Feature-Scale Profile Simulator

Bob Walker
28 October 1999

Brian Kendrick, Joel Kress,
Denise George, Andrew Kuprat, Tinka Gammel,
Dave Hanson, Art Voter
LANL

Mike Coltrin, Pauline Ho
SNL

TopoSim-3D

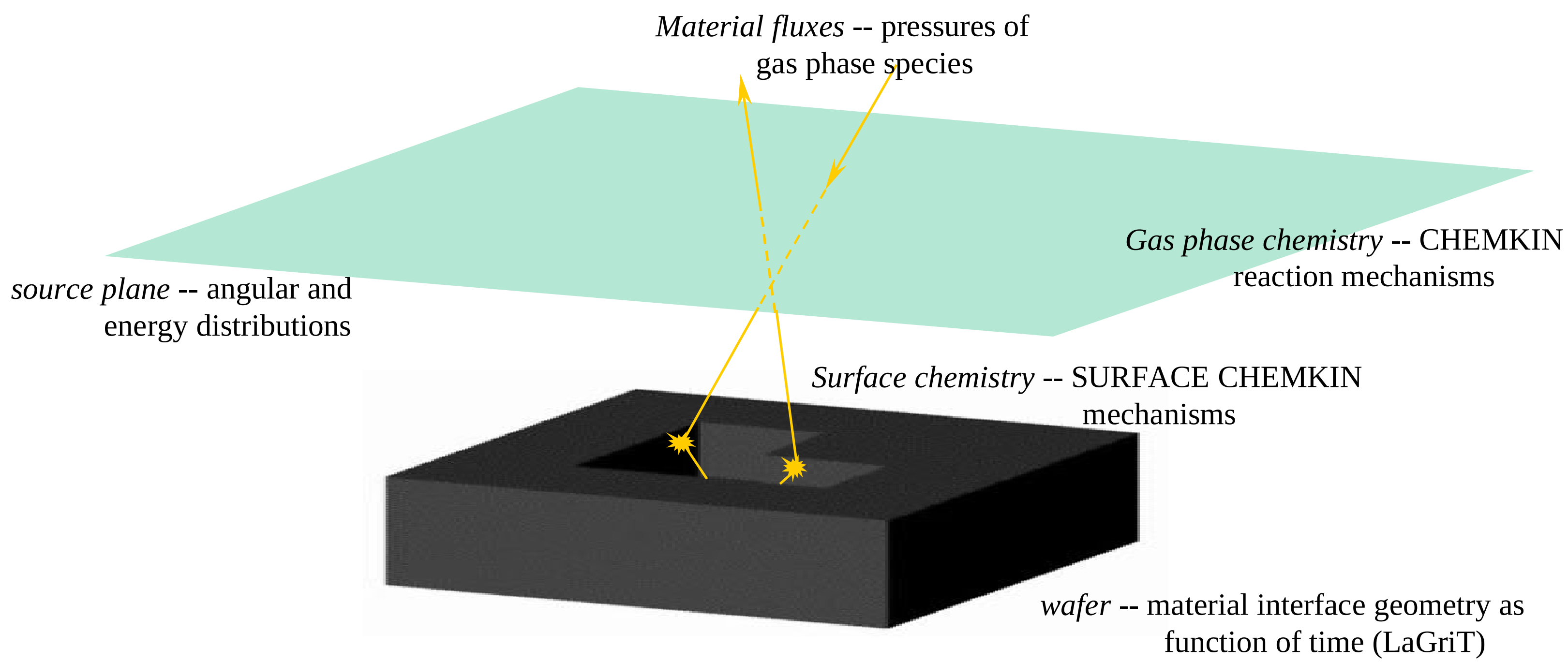
Status -- October 1999

- Code Status, Capabilities
- Example Calculations
  - 3D geometry effects
    - overhang geometries
    - deposition near elbows
    - deposition in damascene structures
  - Bridging to the atomistic scale
  - Bridging to the mesoscopic scale

TopoSim-3D

Code Status 1

TopoSim-3D is a three-dimensional feature-scale topographic simulator. It treats the time development of material deposition/etch on patterned wafers at low pressures.



TopoSim-3D

Module Capabilities

Material Transport

- Can apply orientation-dependent sticking coefficients from MD
- Multiple reflections allowed, reflected material is emissive
- Iteration to self-consistent chemistry based on limiting models for each species
- Fast visibility determination

Source Model

- Uniform, or array of nozzlets
- Allows specification of angular and/or energy distribution of each species

LaGriT

- Uses volume mesh, unstructured grid
- Can adapt mesh to fields, interface curvature
- Can use multiple materials

CHEMKIN / SURFACE CHEMKIN

- Standard chemical kinetics library and database
- Several mechanisms available for semiconductor applications
- Can define multiple reaction mechanisms (materials)

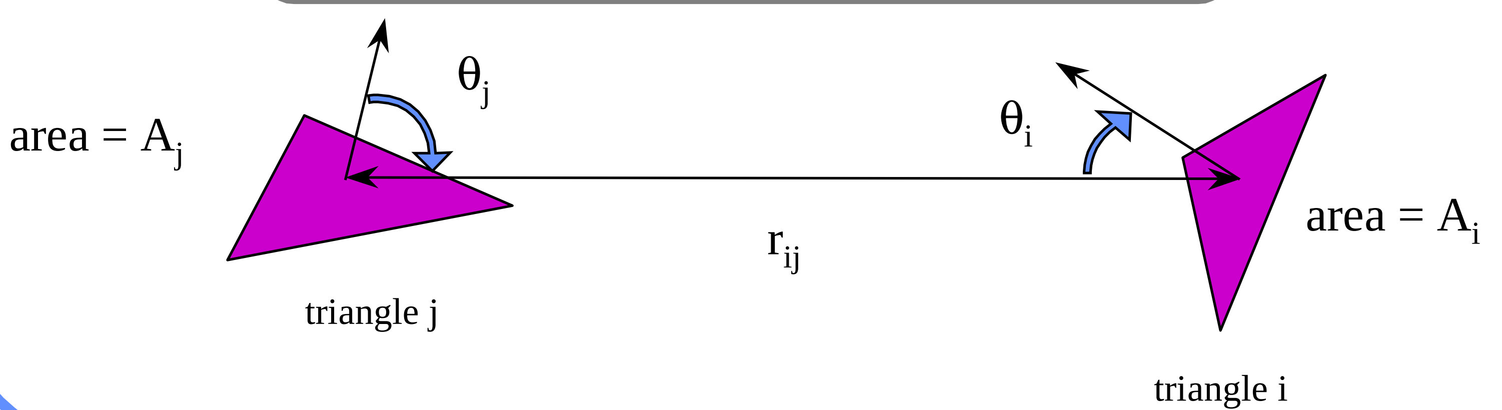
TopoSim-3D

Multiple Scattering

Only a portion of the material that strikes a surface element sticks (or reacts). The rest is rescattered to other parts of the feature. For each interface geometry, we compute a mass transport matrix $\tilde{\boldsymbol{G}}$; each element is the fraction of mass leaving element j that arrives at element I.

$$\tilde{G}_{ij} = (1/\pi)\int_{A_i} dA_i \int_{A_j} \frac{dA_j}{A_j}\,\frac{\cos\theta_i \cdot \cos\theta_j}{r_{ij}^2}$$

Incorporate view factor here, too



TopoSim-3D

Self-Consistent Chemistry

The reaction process at any surface element depends on the site populations of species on the surface, and on the arrival rate of materials transported form the gas phase. Species arriving from the gas phase come directly from the source plane, and from rescattered material from other locations on the interface.

direct flux

flux transport fraction

Flux of species k arriving at triangle i

$$\Phi_{ik}^{+} = \Phi_{ik}^{0} + \sum_{j \neq i} G_{ij}\left(\Phi_{jk}^{+} - R_{jk}\right)$$

reaction rate of species k on triangle j

$$G_{ij} = \tilde{G}_{ij}\left(\frac{A_j}{A_i}\right)$$

Convert mass transport fraction to flux transport fraction

TopoSim-3D

Self-Consistent Chemistry Iteration Schemes -- 1

If we rewrite the rescattering equation as a matrix expression, we have for each column (species) **X** of the flux matrix $\mathbf{\Phi}$ --

$$\mathbf{X} = \mathbf{X}_0 + \mathbf{G}\,(\mathbf{X} - \mathbf{R}(\mathbf{X}))$$

For highly reactive species,

$$X - R(X) \approx 0$$

and so we iterate:

$$X^{(1)} = X_0$$

$$X^{(2)} = X_0 + G(X^{(1)} - R^{(1)})$$

$$X^{(3)} = X_0 + G(X^{(2)} - R^{(2)})$$

$$X^{(4)} = X_0 + G(X^{(3)} - R^{(3)})$$

until $\quad X^{(n+1)} = X^{(n)}$

For low-reactive species,

$$R(X) \approx 0$$

$$R(0) = R(X_0) \quad \cdots \quad R(n) = R(X^{(n)})$$

solve formally for X:

$$X = (1 - G)^{-1}\left[X_0 - G \cdot R\right]$$

then we iterate:

$$X^{(1)} = (1 - G)^{-1}\left[X_0 - G \cdot R^{(0)}\right]$$

$$X^{(2)} = (1 - G)^{-1}\left[X_0 - G \cdot R^{(1)}\right]$$

$$X^{(3)} = (1 - G)^{-1}\left[X_0 - G \cdot R^{(2)}\right]$$

until $\; X^{(n+1)} = X^{(n)}$

TopoSim-3D

Self-Consistent Chemistry Iteration Schemes -- 2

Convergence to self-consistency is accelerated when the reactive flux **R(X)** can be approximated as a fraction *f* of the incident flux **X**. Define also a non-sticking fraction *g* so that $(f + g) = 1$. Then, the original rescattering equation becomes

$$\mathbf{X} = \mathbf{X}_0 + \mathbf{G}\,((f + g)\mathbf{X} - \mathbf{R}(\mathbf{X}))$$

So, for intermediate reactive species,

$$f\,\mathrm{X} - \mathrm{R(X)} \approx 0$$

$$\mathrm{R}^{(0)} = \mathrm{R}(\mathrm{X}_0) \quad \cdots \quad \mathrm{R}^{(n)} = \mathrm{R}(\mathrm{X}^{(n)})$$

solve formally for X:

$$\mathrm{X} = (1 - g\mathrm{G})^{-1}\left[\mathrm{X}_0 + \mathrm{G}\cdot(f\,\mathrm{X} - \mathrm{R})\right]$$

then we iterate:

$$\mathrm{X}^{(1)} = (1 - g\mathrm{G})^{-1}\left[\mathrm{X}_0 + \mathrm{G}\cdot(f\,\mathrm{X}^{(0)} - \mathrm{R}^{(0)})\right]$$

$$\mathrm{X}^{(2)} = (1 - g\mathrm{G})^{-1}\left[\mathrm{X}_0 + \mathrm{G}\cdot(f\,\mathrm{X}^{(1)} - \mathrm{R}^{(1)})\right]$$

$$\mathrm{X}^{(3)} = (1 - g\mathrm{G})^{-1}\left[\mathrm{X}_0 + \mathrm{G}\cdot(f\,\mathrm{X}^{(2)} - \mathrm{R}^{(2)})\right]$$

until $\mathrm{X}^{(n+1)} = \mathrm{X}^{(n)}$

TopoSim-3D

Code Status 2

- Versions Distributed to:
  - Motorola
  - Sandia National Laboratory
  - Intel
  - IBM

- Code Ported to platforms:
  - HP (f77 and f90)
  - SGI
  - IBM
  - Sun

- Enhanced capabilities:
  - Choice of surface moving algorithms
  - 10X improvement in speed of visibility determinations using volume mesh connectivity information
  - Establish interface between LaGriT and SURFACE CHEMKIN materials
  - Establish interface to MD calculations
  - Improved self-consistent chemistry for intermediate-reactive species

TopoSim-3D

Future Plans

Continue development in three task areas

<u>Interface to MD</u>

- Add sputter yield
- Specular reflections
- Particle tracking (MC)

<u>Grain Growth Models</u>

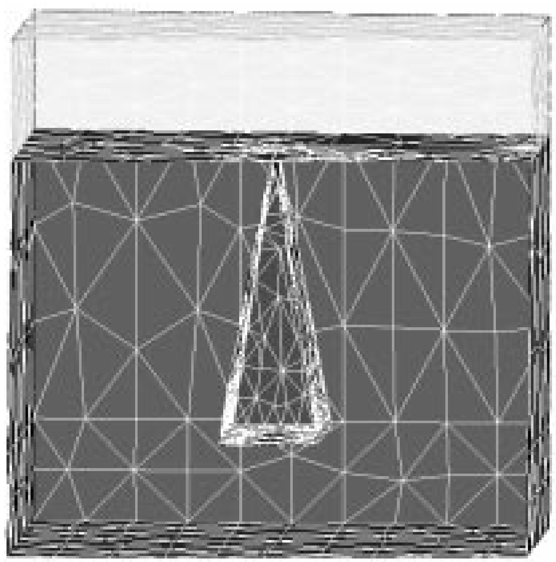
- Refine code interface
- Enhance growth physics

<u>Application to Plasma Etch</u>

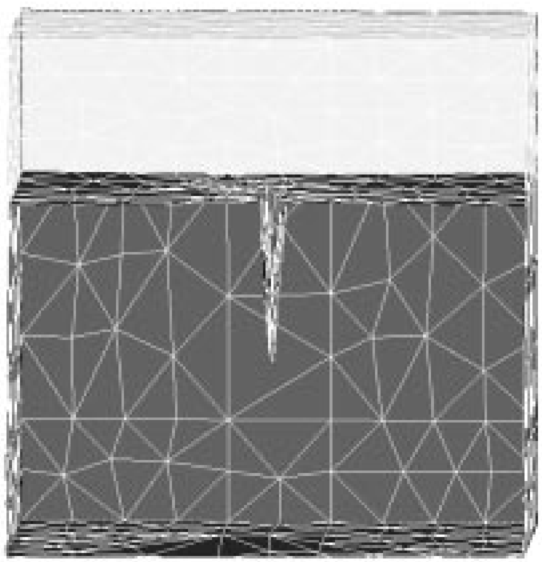
- Add sheath physics
- Use MD interface
- Test new chemistries

TopoSim-3D

Long-Time
Trench Fills



Silane chemistry

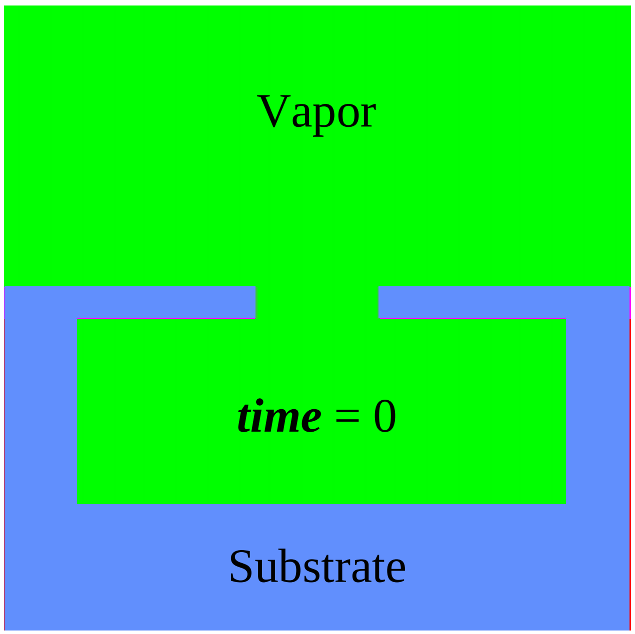


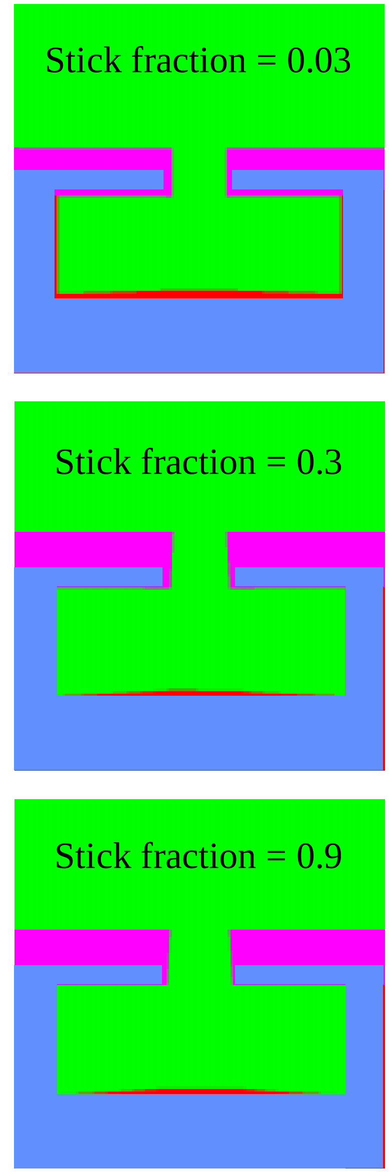
TEOS chemistry

These are cutaway views of deposition into a trench whose original aspect ratio was 1.5, at a time just prior to closure at the top of the trench. On the left, silane deposition chemistry is modeled, and on the right, TEOS chemistry is modeled. The higher sticking fraction for silane chemistry produces a large triangular void, while the low sticking fraction for TEOS chemistry produces a much more conformal deposition profile, with no void formation in the (soon-to-be) filled trench.

TopoSim-3D

Deposition into an Overhang Structure

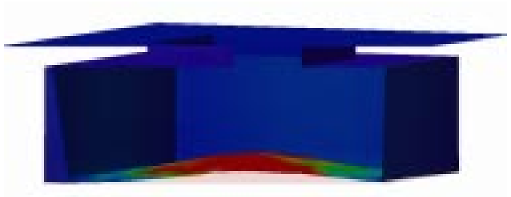




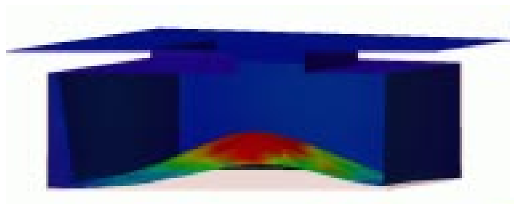
Illustrates deposition into overhang structures for different sticking fractions. As the sticking fraction increases, less material is deposited on the roof and side walls of the internal structure.

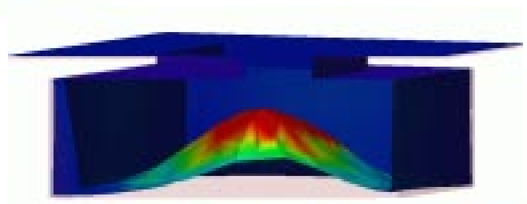
TopoSim-3D

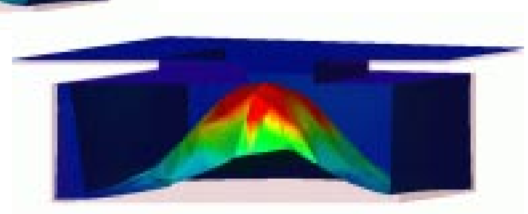
Cutaway View of Deposition into an Overhang Structure (vs. time)



time →







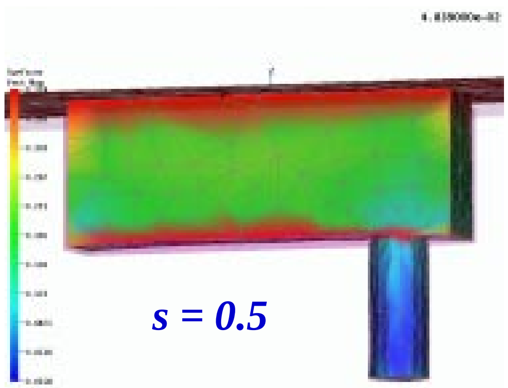
Sticking fractions:

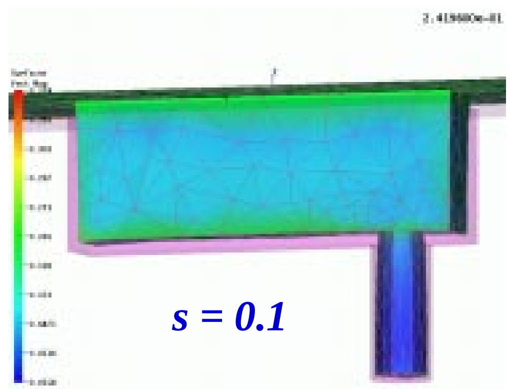
- *mask* = 0.05
- *cavity* = 0.60

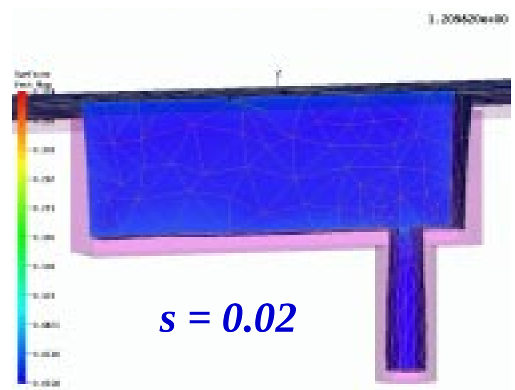
At each time step, the vapor/substrate interface is rendered in the color of the local node velocity. The fastest growing portions of the interface are colored red, and the slowest are blue. Green/yellow colors are intermediate. The t=0 interface is rendered transparent (pink), and can be seen at the edges of the colored parts of the interface.

TopoSim-3D

View of Deposition into a Damascene Structure (vs. sticking coefficient)



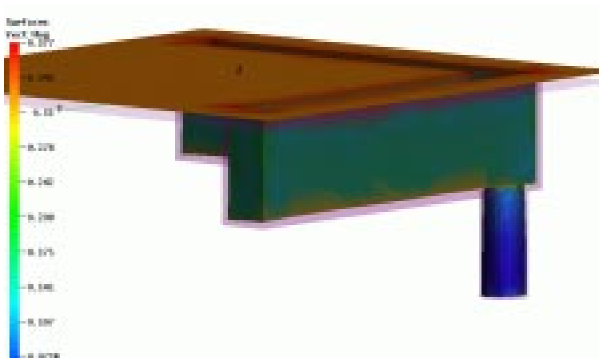




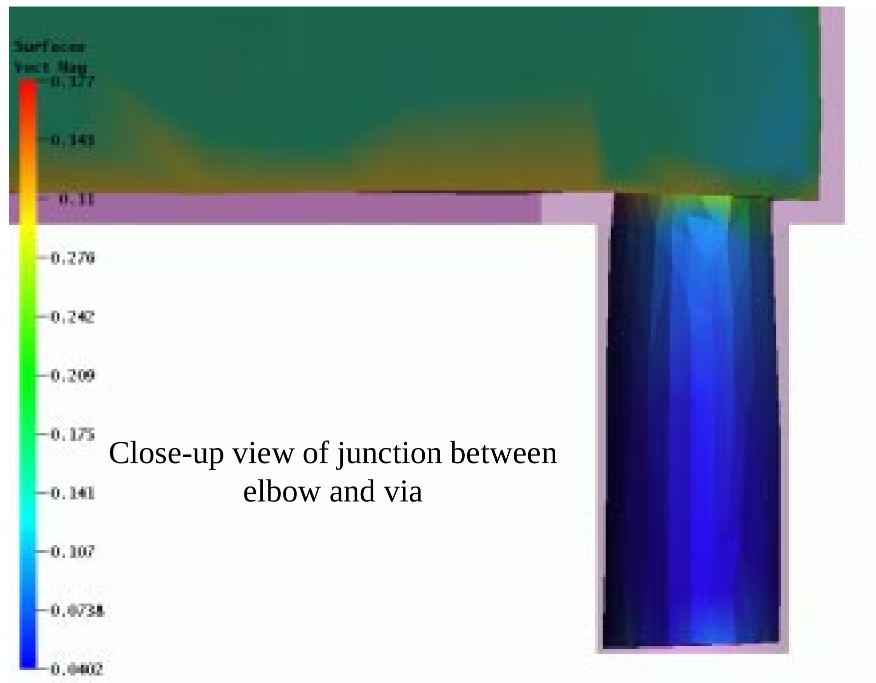
- Aspect ratios: trench = 2, via = 2
- Original vapor/substrate interface is transparent (pink)
- Red color => fastest moving nodes
- Blue color => slowest nodes
- Deposition on surface field = 0.2 microns

TopoSim-3D

View of Deposition into an Elbow/via Structure



Simulation volume = 2 micron cube



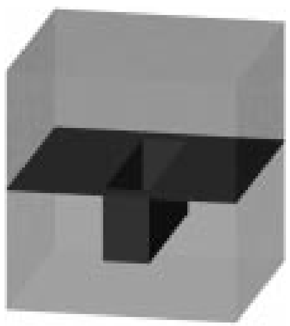
Close-up view of junction between elbow and via

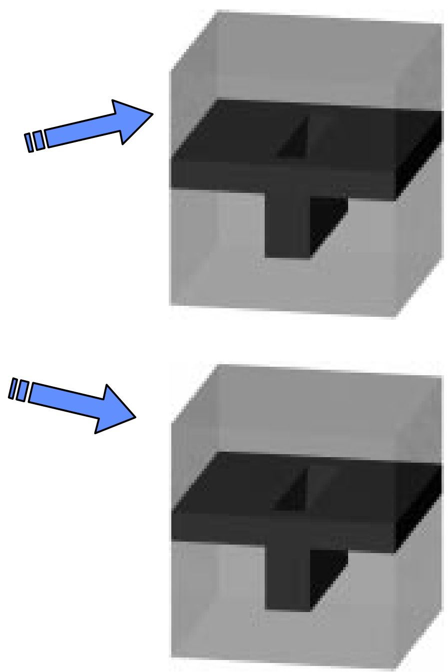
- Aspect ratios: trench = 2, via = 2
- Sticking fraction: s = 0.2
- Angular distribution: cosine power = 8
- Red => fastest nodes
- Blue => slowest nodes

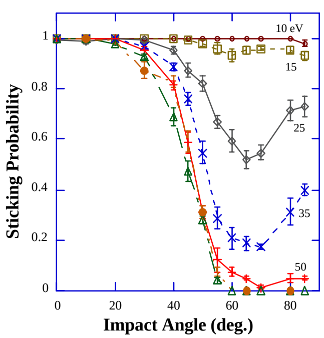
TopoSim-3D

Bridging the Length Scale: Atomistic to Mesoscopic

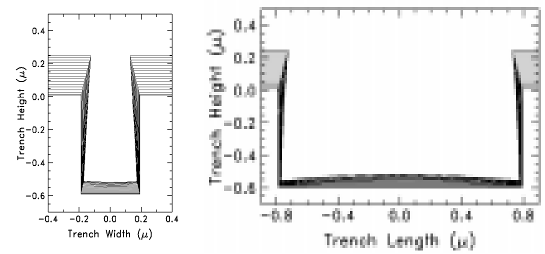
Example shows importance of using atomistic simulation data on the deposition profile of Cu in a trench fill simulation.



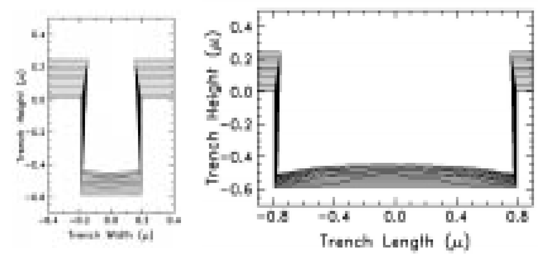




Deposition using constant sticking probability (= 1.0)



Profile after 0.25μ Cu deposited on top surface

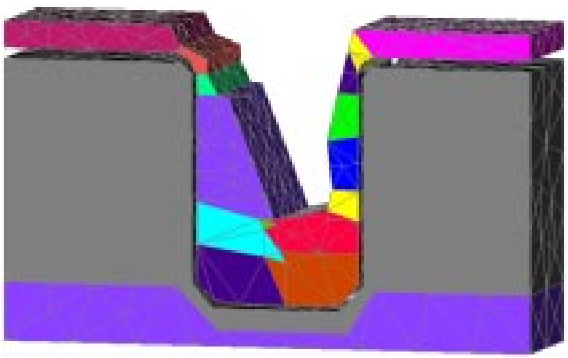


Deposition at 50eV using atomistic sticking probability

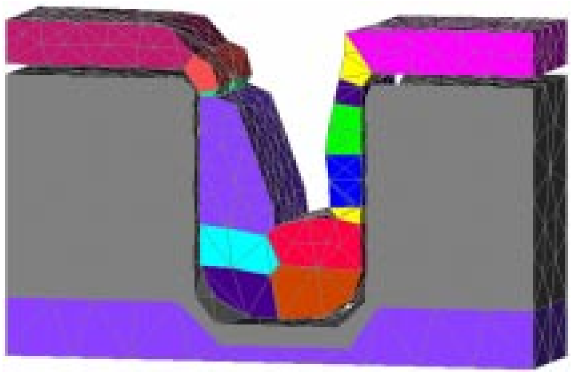
TopoSim-3D

Coupling to Grain Growth
Tinka Gammel, Andrew Kuprat (LANL T-1)
(started September 1998)

- Each grain a different material to SURFACE CHEMKIN and LaGriT
- TopoSim-3D and Grain3D exchange data through external files
  - -- TopoSim-3D generates triangle velocity vectors, pass to Grain3D
  - -- Grain3D advances time, generates new mesh object
- Images illustrate grain evolution during deposition



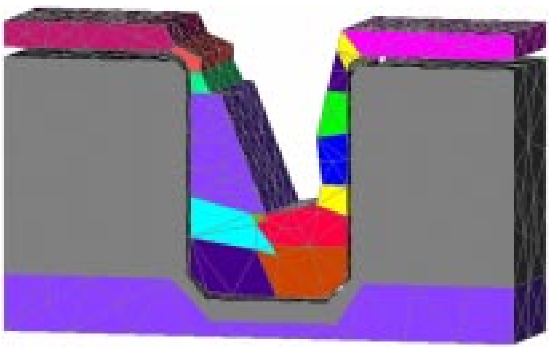
***time* = 0**



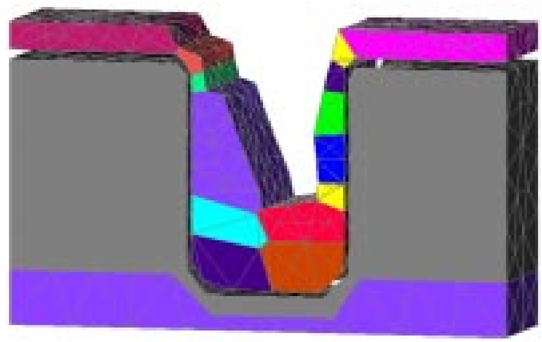
***time* = 6 ms**

TopoSim-3D

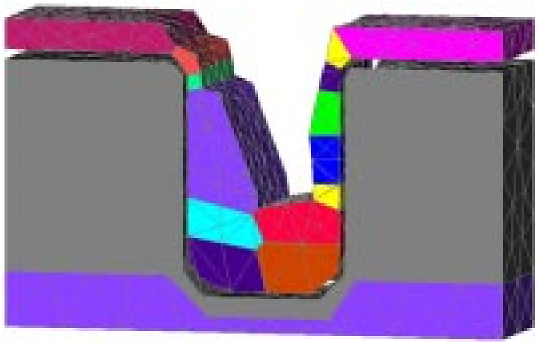
Grain Growth During Deposition



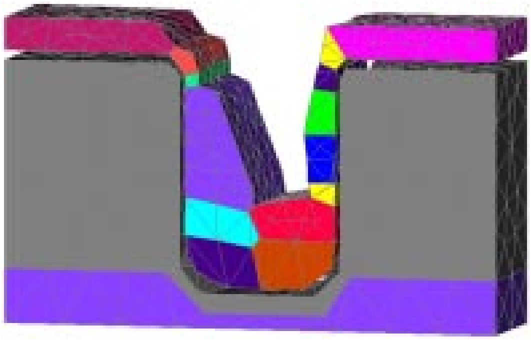
0 ms



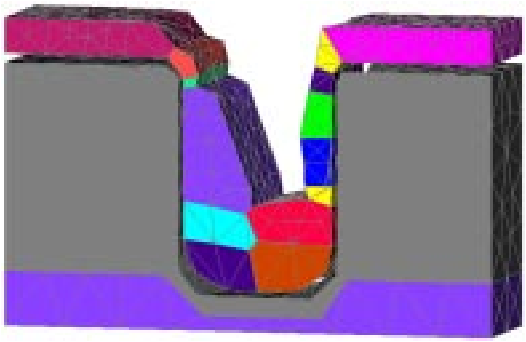
1 ms



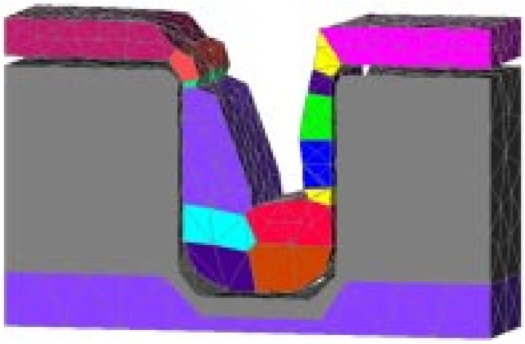
2 ms



3 ms



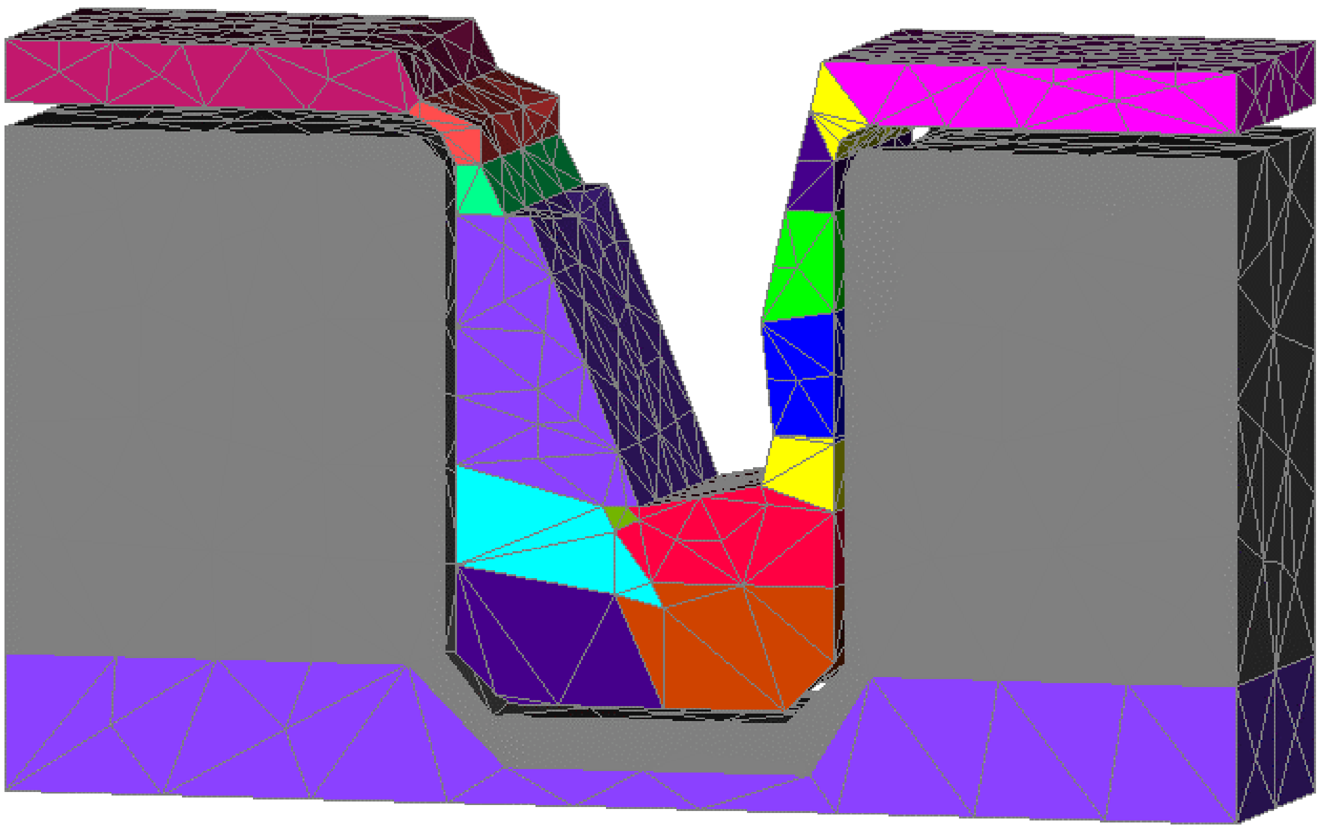
4 ms



5 ms

TopoSim-3D

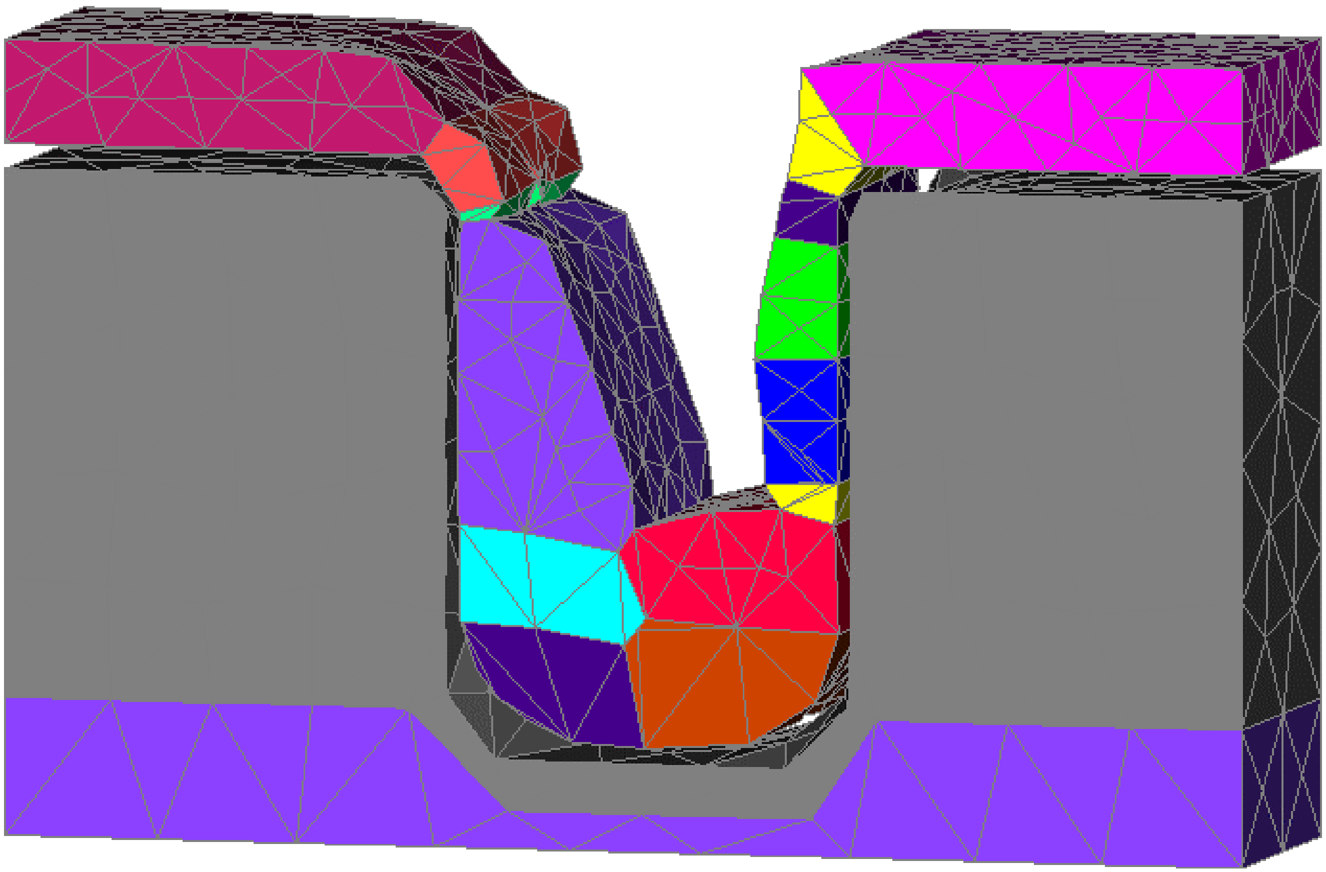
Grain Growth
During Deposition



time = 0

TopoSim-3D

Grain Growth
During Deposition



time = 6 ms